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=> fil reg

FILE 'REGISTRY' ENTERED AT 08:32:31 ON 05 SEP 2000
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STRUCTURE FILE UPDATES:    4 SEP 2000  HIGHEST RN 288141-13-9
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TSCA INFORMATION NOW CURRENT THROUGH JANUARY 11, 2000

  Please note that search-term pricing does apply when
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Structure search limits have been increased.  See HELP SLIMIT
for details.

=> d sta que l20

L20           1 SEA FILE=REGISTRY ABB=ON  PLU=ON  (LMYPTYLK)/SQEP


=> d his l20-l22


     (FILE 'REGISTRY' ENTERED AT 08:24:03 ON 05 SEP 2000)
                E 'LEU-MET-TYR-PRO-THR-TYR-LEU-LYS'/SQEP
L20           1 S E3
                E 'AIB-MET-TYR-PRO-THR-TYR-AIB-LYS'/SQEP
                E 'LEU-MET-TYR-PRO-THR-TYR-AIB-LYS'/SQEP
                E 'AIB-MET-TYR-PRO-THR-TYR'/SQEP
                E 'LEU-MET-TYR-PRO-THR-TYR'/SQEP

     FILE 'HCAOLD' ENTERED AT 08:30:44 ON 05 SEP 2000
L21           0 S L20

     FILE 'HCAPLUS' ENTERED AT 08:30:49 ON 05 SEP 2000
L22           4 S L20

=> d l20 sqide can


L20  ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2000 ACS
RN   120550-85-8  REGISTRY
CN   L-Lysine, N2-[N-[N-[N-[1-[N-(N-L-leucyl-L-methionyl)-L-tyrosyl]-L-prolyl]-
     L-threonyl]-L-tyrosyl]-L-leucyl]- (9CI)  (CA INDEX NAME)
FS   PROTEIN SEQUENCE; STEREOSEARCH
SQL  8

SEQ      1 LMYPTYLK
           ========
HITS AT:   1-8
MF   C50 H77 N9 O12 S
SR   CA
LC   STN Files:   CA, CAPLUS, CHEMCATS, TOXLIT, USPATFULL

Absolute stereochemistry.
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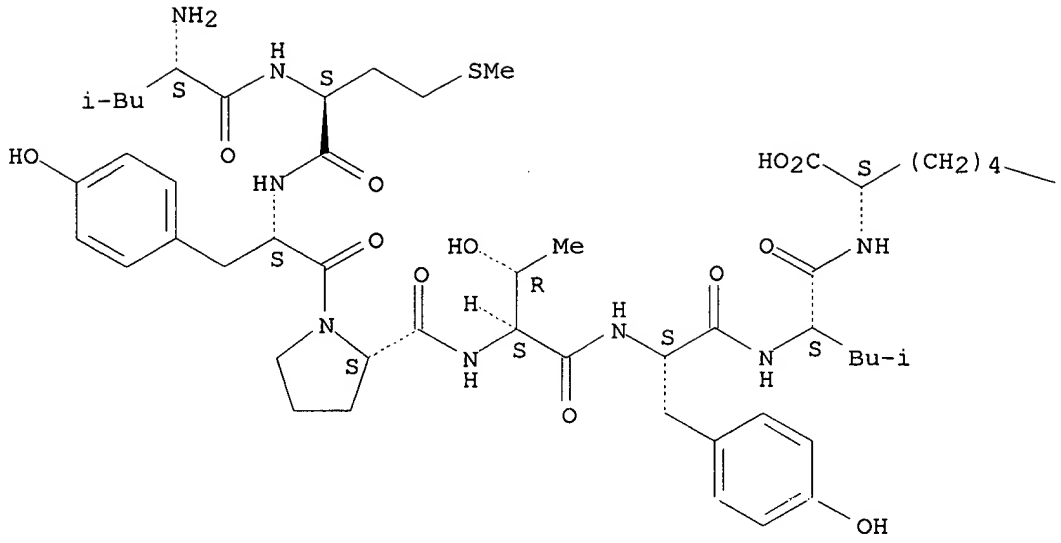
Point of Contact:
Jan Delaval
Librarian-Physical Sciences
CM1 1E01 Tel: 308-4498

PAGE 1-A



PAGE 1-B

4 REFERENCES IN FILE CA (1967 TO DATE)
4 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 119:217605

REFERENCE 2: 116:249474

REFERENCE 3: 114:95463

REFERENCE 4: 110:206193

=> fil hcaplus

FILE 'HCAPLUS' ENTERED AT 08:32:46 ON 05 SEP 2000

FILE COVERS 1967 - 5 Sep 2000 VOL 133 ISS 11
FILE LAST UPDATED: 4 Sep 2000 (20000904/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

This file supports REG1stRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

Now you can extend your author, patent assignee, patent information, and title searches back to 1907. The records from 1907-1966 now have this searchable data in CAOLD. You now have electronic access to all of CA: 1907 to 1966 in CAOLD and 1967 to the present in HCAPLUS on STN.

=> d all tot l22

L22 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2000 ACS
AN 1993:617605 HCAPLUS
DN 119:217605
TI The entire vasoactive intestinal polypeptide molecule is required for the activation of the vasoactive intestinal polypeptide receptor: Functional and binding studies on opposum internal anal sphincter smooth muscle
AU Chakder, Sushanta; Rattan, Satish
CS Dep. Med., Thomas Jefferson Univ., Philadelphia, PA, USA
SO J. Pharmacol. Exp. Ther. (1993), 266(1), 392-9
CODEN: JPETAB; ISSN: 0022-3565
DT Journal
LA English
CC 2-2 (Mammalian Hormones)
AB Because no significant information exists regarding the structure-activity of VIP to gut smooth muscle, the authors performed functional studies in vitro on opossum internal anal sphincter (IAS) smooth muscle strips and supplemented them with binding studies to assess the ability of VIP, its fragments, and analogs to inhibit [125I]VIP binding to IAS smooth muscle membranes. Binding of radiolabeled VIP to its receptor was specific, saturable, and time- and temp.-dependent. Of all the substances tested, VIP was the most potent in causing a fall in the resting tension of the IAS and inhibiting [125I]VIP binding. VIP 2-28, VIP 10-28 and the putative VIP antagonists [4Cl-D-Phe6,Leu17]VIP (VIP analog) and (N-Ac-Tyr1,D-Phe2)-growth hormone-releasing factor [GRF] (1-29)-NH2 (GRF analog) caused significant inhibition of [125I]VIP binding, but had only minimal effect on the resting tension of the IAS. VIP 9-18 and VIP 1-12 had neither any significant effect nor inhibition of receptor binding. The rank order of potencies nor inhibition of receptor binding. The rank order of potencies for inhibition of binding was VIP > VIP analog > VIP 10-18 = VIP 2-28 > GRF analog > peptide histidine isoleucine > VIP 9-18. The IC50 values for VIP, VIP analog, VIP 10-28, VIP 2-28, GRF analog, and peptide histidine isoleucine were 9.6 .times. 10-9, 1.6 .times. 10-7, 5.5 .times. 10-7, 6.2 .times. 10-7, 1.2 .times. 10-8, and 1.2 .times. 10-5 M, resp. The full action of VIP is critically dependent upon the integrity of the entire VIP mol. However, only the C-terminal part of the mol. is needed for binding to the receptor. These studies provide previously unknown information on selective VIP receptor antagonists and VIP receptor characterization.
ST VIP receptor activation
IT Molecular structure-biological activity relationship
(digestive tract-relaxing, of VIP analogs and fragments)
IT Digestive tract
(relaxation of smooth muscles of, by VIP analogs and fragments, structure in relation to)
IT Receptors
RL: BIOL (Biological study)
(vasoactive intestinal polypeptide, VIP analogs and fragments binding by, structure in relation to)
IT Molecular structure-biological activity relationship
(vasoactive intestinal polypeptide receptor-binding, of VIP analogs and fragments)

IT 40077-57-4, Vasoactive intestinal octacosapeptide (pig) 69856-17-3
80458-29-3, PHI-27 91409-16-4, VIP-2-28 93965-89-0 102805-45-8
120550-85-8 120928-03-2, VIP-1-12 150503-16-5, VIP-9-18
RL: BIOL (Biological study)
(digestive tract smooth muscle relaxation by and receptor binding of, structure in relation to)

L22 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2000 ACS
AN 1992:249474 HCAPLUS
DN 116:249474
TI Vasoactive intestinal polypeptide peptide antagonists
IN Gozes, Illana; Brenneman, Douglas; Fridkin, Mati; Moody, Terry
PA United States Dept. of Health and Human Services, USA
SO U. S. Pat. Appl., 35 pp. Avail. NTIS Order No. PAT-APPL-7-620,410.
CODEN: XAXXAV
DT Patent
LA English
CC 2-6 (Mammalian Hormones)
Section cross-reference(s): 1
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 620410	A0	19920215	US 1990-620410	19901130
US 5217953	A	19930608		

AB Peptide antagonists of vasoactive intestinal polypeptide (VIP) are disclosed. The octomer Leu-Met-Tyr-Pro-Thr-Tyr-Leu-Lys, as well as a VIP-neurotensin hybrid, inhibited VIP-stimulated sexual behavior in rats. The VIP-neurotensin hybrid antagonist was tested for ability to inhibit nonsmall cell lung cancer cell lines; this antagonist inhibited colony formation of cell lines NCI-H522 and NCI-H838, but not NCI-H1246. Seq ID 3
ST vasoactive intestinal polypeptide peptide antagonist; neurotensin VIP hybrid VIP antagonist; lung cancer inhibitor VIP antagonist
IT Sexual behavior
(vasoactive intestinal polypeptide antagonist effect on vasoactive intestinal polypeptide-induced, in rat)
IT Peptides, biological studies
RL: BIOL (Biological study)
(vasoactive intestinal polypeptide antagonists)
IT Neoplasm inhibitors
(lung non-small-cell carcinoma, vasoactive intestinal polypeptide-neurotensin hybrid)
IT Lung, neoplasm
(non-small-cell carcinoma, inhibitors, vasoactive intestinal polypeptide-neurotensin hybrid)
IT Receptors
RL: BIOL (Biological study)
(vasoactive intestinal polypeptide, in lung cancer cell lines, vasoactive intestinal polypeptide binding to, vasoactive intestinal polypeptide antagonist activity in relation to)
IT 39379-15-2D, Neurotensin, vasoactive intestinal polypeptide hybrids
RL: BIOL (Biological study)
(as vasoactive intestinal polypeptide antagonist)
IT 37221-79-7, Vasoactive intestinal polypeptide
RL: BIOL (Biological study)
(peptide antagonists of)
IT **120550-85-8**
RL: BAC (Biological activity or effector, except adverse); BIOL (Biological study)
(vasoactive intestinal polypeptide antagonist activity of)

L22 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2000 ACS
AN 1991:95463 HCAPLUS
DN 114:95463
TI High affinity receptors for vasoactive intestinal peptide on a human glioma cell line
AU Nielsen, Finn C.; Gammeltoft, Steen; Westermark, Bengt; Fahrenkrug, Jan

CS Dep. Clin. Chem., Bispebjerg Hosp., Copenhagen, DK-2400, Den.
SO Peptides (Fayetteville, N. Y.) (1990), 11(6), 1225-31
CODEN: PPTDD5; ISSN: 0196-9781
DT Journal
LA English
CC 2-6 (Mammalian Hormones)
AB VIP bound with high affinity (Kd 0.13 nmol/L) to receptors on the human glioma cell line U-343 MG Cl 2:6. The receptors bound the related peptides helodermin, PHM, and secretin with 10, 400 and 5000 times lower affinity, resp. Deamidated VIP (VIP-COOH) and [des-His1]VIP bound with 10 and 100 times lower affinity. The fragment VIP(7-28) displaced 25% of the receptor-bound 125I-VIP whereas VIP(16-28) and VIP(1-22-NH2) were inactive. The binding of 125I-VIP could be completely inhibited by 10 .mu.mol/L of the antagonists [N-Ac-Tyr1,D-Phe2]GRF(1-29)-NH2, [pCl-D-Phe6,Leu17]VIP and VIP(10-28); in contrast, the antagonist L-8-K was inactive. Affinity labeling showed that VIP bound to proteins with Mr's of 75 kDa, 66 kDa, and 50 kDa, resp. Following binding, the peptide was rapidly internalized, and at steady-state only 20% of cell-assocd. 125I-VIP was bound to receptors on the cell surface. The internalized 125I-VIP was completely degraded to 125I-tyrosine which was released from the cells. Degrdn. of internalized 125I-VIP was reduced by chloroquine, phenantroline, and pepstatin-A. Surface binding and internalization of 125I-VIP was increased 3 times by phenantroline, and pepstatin-A caused a 5 times increased in surface binding. Chloroquine reduced surface-bound 125I-VIP, but caused retention of internalized 125I-VIP.
ST glioma VIP receptor internalization
IT Neuroglia
(VIP receptors on human)
IT Receptors
RL: PROC (Process)
(for VIP, on glioma cell line of humans, processing of)
IT Biological transport
(internalization, of VIP receptors, by human glioma)
IT 87171-19-5, VIP(16-28) 132333-38-1, VIP(1-22-amide)
RL: BIOL (Biological study)
(VIP binding by receptor in human glioma in presence of)
IT **120550-85-8**
RL: BIOL (Biological study)
(VIP binding by receptor of human glioma in presence of)
IT 69856-17-3 93965-89-0 102805-45-8
RL: BIOL (Biological study)
(VIP binding by receptor on human glioma cell line inhibition by)
IT 40077-61-0 60703-95-9, VIP-COOH 91409-16-4, [Des-His1]VIP
RL: PROC (Process)
(binding of, by VIP receptor of glioma of humans)
IT 37221-79-7, VIP
RL: BIOL (Biological study)
(receptors for, of glioma cell line of humans, processing of)

L22 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2000 ACS
AN 1989:206193 HCAPLUS
DN 110:206193
TI High-affinity receptors for vasoactive intestinal peptide on human myeloma cells
AU Finch, Rosalynde J.; Sreedharan, Sunil P.; Goetzl, Edward J.
CS Med. Cent., Univ. California, San Francisco, CA, 94143-0724, USA
SO J. Immunol. (1989), 142(6), 1977-81
CODEN: JOIMA3; ISSN: 0022-1767
DT Journal
LA English
CC 2-6 (Mammalian Hormones)
AB Cultured human myeloma cells of the U266 line and leukemic T cells of the Jurkat line bound synthetic [125I]Tyr10-VIP 1-28 ([125I]VIP1-28) specifically and with an affinity similar to that of neuroendocrine cells. Specific binding reached equil. after 2 h at 22.degree. for both myeloma cells and T cells, attained a max. of 57-71% of total binding, and was

reversed in 1.5-3 h by an excess of nonradioactive VIP1-28. Analyses of the ligand concn.-dependence of binding of [125I]VIP1-28 revealed a mean Kd of 7.6 nM for a mean of 41,207 receptors per myeloma cell and 5.2 nM for 12,266 receptors per T cell. The relative affinity of binding of mast cell-derived VIP10-28 free acid and synthetic analogs suggested differences in specificity between lymphocyte and neuroendocrine receptors. Distinct sets of receptors thus appear to mediate the effects of VIP on functions of both antibody-producing cells and T cells.

ST VIP receptor myeloma cell lymphocyte

IT Myeloma
(VIP receptors of human in)

IT Receptors
RL: BIOL (Biological study)
(for VIP, of myeloma cells and T-lymphocytes of humans)

IT Lymphocyte
(T-, VIP receptors of human in)

IT 93965-89-0 115722-31-1 **120550-85-8**
RL: BIOL (Biological study)
(VIP binding by receptors of myeloma cells antagonism by)

IT 37221-79-7, Vasoactive intestinal polypeptide
RL: BIOL (Biological study)
(receptors for, of myeloma cells and T-lymphocytes of humans)

=> d his l1-l17

(FILE 'HOME' ENTERED AT 08:19:46 ON 05 SEP 2000)
SET COST OFF

FILE 'HCAPLUS' ENTERED AT 08:19:57 ON 05 SEP 2000
E MUKHERJEE R/AU
L1 251 S E3-E7,E18
E JAGGI M/AU
L2 9 S E3,E4,E6
E PRASAD S/AU
L3 605 S E3-E39
E PRASAD SUDHAN/AU
L4 9 S E4
E BURMAN A/AU
L5 5 S E4-E5,E7,E8
L6 875 S L1-L5
L7 6 S L6 AND 34/SC,SX
L8 17 S L6 AND ?PEPTIDE?
L9 0 S L6 AND BOMBESIN
L10 2 S L6 AND DXG
L11 2 S L10 AND L7,L8
L12 2 S L1 AND L2-L5
L13 1 S L2 AND L3-L5
L14 1 S L3,L4 AND L5
L15 2 S L12-L14
L16 1 S L15 AND 63/SC,SX
L17 3 S L11,L16

=> d all tot l17

L17 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2000 ACS
AN 2000:573679 HCAPLUS
TI Antiangiogenic drugs
IN **Mukherjee, Rama; Jaggi, Manu; Prasad, Sudhanand; Burman, Anand C.**; Rajendran, Praveen; Mathur, Archana; Singh, Anu T.
PA National Institute of Immunology, India; Dabur Research Foundation; Cord, Janet, I.
SO PCT Int. Appl., 42 pp.

CODEN: PIXXD2
DT Patent
LA English
IC ICM A61K038-00
ICS A61K038-02; C07K005-00; C07K007-00
CC **63** (Pharmaceuticals)
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000047221	A1	20000817	WO 2000-US3559	20000211

PI
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRAI US 1999-248381 19990211
AB The invention relates to the use of peptides individually or in combination, for treating and/or preventing angiogenesis. It also relates to the use of peptide analogs or a combination of peptides referred to as MuJ-7 as anticancer drugs in restricting the tumor growth and spread by inhibiting tumor angiogenesis. MuJ-7, in addition inhibits metastasis through its antiangiogenic activity in all cancers. The invention also relates to a pharmaceutical composition containing either individual peptides or in combination, and methods of treatment of human beings and animals for curing and/or preventing angiogenesis.
RE.CNT 8
RE
(1) Bogden; US 5217955 A 1993
(2) Coy; US 5410019 A 1995 HCAPLUS
(3) Danesi; Metabloism 1996, V45(8, Suppl 1), P49
(4) Gozes; US 5565424 A 1996
(5) Hanahan; Cell 1996, V86, P353 HCAPLUS
(6) Kim; US 5552520 A 1996 HCAPLUS
(7) The Administrators Of The Tulane Educational Fund; WO 9639161 A1 1996 HCAPLUS
(8) Woltering; Journal of Surgical Research 1991, V50(3), P245 HCAPLUS

L17 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2000 ACS
AN 1996:678144 HCAPLUS
DN 125:326338
TI Conformation-activity correlations for chemotactic **tripeptide** analogs incorporating dialkyl residues with linear and cyclic alkyl sidechains at position 2
AU **Prasad, Sudhanand**; Rao, R. Balaji; Bergstrand, Hakan; Lundquist, Britta; Becker, Elmer L.; Balaram, P.
CS Molecular Biophysics Unit, Indian Institue Science, Bangalore, India
SO Int. J. Pept. Protein Res. (1996), 48(4), 312-318
CODEN: IJPPC3; ISSN: 0367-8377
DT Journal
LA English
CC 15-10 (Immunochemistry)
AB Five stereochem. constrained analogs of the chemotactic **tripeptide** incorporating 1-aminocycloalkane-1-carboxylic acid (Acnc) and .chi.,.chi.-dialkylglycines (Deg, diethylyglycine; Dpg, n,n-dipropylglycine and Dbg, n,n-dibutylglycine) at position 2 have been synthesized. NMR studies of **peptides** For-Met-Xxx-Phe-OMe (Xxx=Ac7c I; Ac8c, II; Deg, III; Dpg, IV and Dbg, V; For, formyl) establish that **peptide** with cycloalkyl residues, I and II, adopt folded .beta.-turn conformations in CDCl3 and (CD3)2SO. In contrast, analogs with linear alkyl sidechains, III-V, favor fully extended (C5) conformations in soln. **Peptides** I-V exhibit high activity in inducing .beta.-glucosaminidase release from rabbit neutrophils, with ED50

values ranging from 1.4-8.0 x 10-11M. In human neutrophils the **Dxg peptides** III-V have ED50 values ranging from 2.3 x 10-10 M, with the activity order being V>IV>III. While **peptides** I-IV are less active than the parent, For-Met-Leu-Phe-OH, in stimulating histamine release from human basophils, the Dbg **peptide** V is appreciably more potent, suggesting its potential utility as a probe for formyl **peptide** receptors.

ST chemotactic **tripeptide** conformation activity correlation

IT Basophil
Neutrophil
(conformation-activity correlations for chemotactic **tripeptide** analogs incorporating dialkyl residues with linear and cyclic alkyl sidechains at position 2)

IT **Peptide** receptors
Receptors
RL: BPR (Biological process); BIOL (Biological study); PROC (Process)
(1-(N-formylmethionine)-**peptide**, conformation-activity correlations for chemotactic **tripeptide** analogs incorporating dialkyl residues with linear and cyclic alkyl sidechains at position 2)

IT Molecular structure-biological activity relationship
(chemotactic, conformation-activity correlations for chemotactic **tripeptide** analogs incorporating dialkyl residues with linear and cyclic alkyl sidechains at position 2)

IT 51-45-6, Histamine, biological studies 9012-33-3
RL: BPR (Biological process); BIOL (Biological study); PROC (Process)
(conformation-activity correlations for chemotactic **tripeptide** analogs incorporating dialkyl residues with linear and cyclic alkyl sidechains at position 2)

IT 127291-39-8P 136427-57-1P 181701-83-7P 183429-69-8P 183429-77-8P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(conformation-activity correlations for chemotactic **tripeptide** analogs incorporating dialkyl residues with linear and cyclic alkyl sidechains at position 2)

IT 2488-15-5 2577-90-4 6141-45-3 70974-26-4 87113-23-3 183429-63-2
183429-68-7
RL: RCT (Reactant)
(conformation-activity correlations for chemotactic **tripeptide** analogs incorporating dialkyl residues with linear and cyclic alkyl sidechains at position 2)

IT 138123-33-8P 183429-61-0P 183429-62-1P 183429-65-4P 183429-66-5P
183429-67-6P 183429-70-1P 183429-71-2P 183429-72-3P 183429-74-5P
183429-75-6P 183429-76-7P 183429-78-9P 183429-79-0P 183429-80-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(conformation-activity correlations for chemotactic **tripeptide** analogs incorporating dialkyl residues with linear and cyclic alkyl sidechains at position 2)

L17 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2000 ACS
AN 1995:406397 HCAPLUS
DN 122:315080
TI Contrasting solution conformations of **peptides** containing .alpha.,.alpha.-dialkylated residues with linear and cyclic side chains
AU **Prasad, Sudhanand**; Rao, R. Balaji; Balaram, P.
CS Dep. Chem., Banaras Hindu Univ., Varanasi, 221 005, India
SO Biopolymers (1995), 35(1), 11-20
CODEN: BIPMAA; ISSN: 0006-3525
DT Journal
LA English
CC **34-3** (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 22

AB The conformational properties of five **peptides** Boc-Ala-X-Ala-OMe [Boc = Me3CO2C: X = diethylglycine (I), dipropylglycine (II), dibutylglycine (III), 1-aminocyclohexane-1-carboxylic acid (IV), and 1-aminocycloheptane-1-carboxylic acid (V)] contg. acyclic .alpha.,.alpha.-dialkylglycine (**Dxg**) and 1-aminocycloalkane-1-carboxylic acid (Acnc) residues were studied in soln. by NMR and CD.

Delineation of solvent-shielded NH groups have been achieved by solvent and temp. dependence of NH chem. shifts in CDCl3 and (CD3)2SO and by paramagnetic radical induced line broadening in **peptide** III. In **Dxg**-contg. **peptides** I-III, the order of solvent exposure of NH groups is Ala1 > Ala3 > Dxg2, whereas in Acnc-contg. **peptides** IV and V, the order of solvent exposure of NH groups is Ala1 > Acnc2 > Ala3. The NMR results suggest that Acnc-contg. **peptides** IV and V adopt folded .beta.-turn conformations with Ala1 and Acnc2 occupying i + 1 and i + 2 positions. In contrast, **Dxg** -contg. **peptides** I-III favor extended C5 conformations. The conformational differences in the two series are clearly borne out in CD studies. The soln. conformations of **Dxg**-contg. **peptides** I-III are distinctly different from the .beta.-turn structure obsd. in crystals. Low temp. NMR spectra recorded immediately after dissoln. of crystals of **peptide** II provide evidence for a structural transition. Introduction of an addnl. hydrogen-bonding function in Boc-Ala-Dpg-Ala-NHMe (VI) results in a stabilization of a consecutive .beta.-turn or incipient 310-helix in soln.

ST conformation dialkylated amino acid **peptide**; aminocycloalkanecarboxylic acid **peptide** conformation; glycine dialkyl **peptide** conformation

IT Conformation and Conformers
(contrasting soln. conformations of **peptides** contg. .alpha.,.alpha.-dialkylglycine and aminocycloalkanecarboxylic acid residues)

IT **Peptides**, preparation
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(dialkylglycine-contg.; contrasting soln. conformations of **peptides** contg. .alpha.,.alpha.-dialkylglycine and aminocycloalkanecarboxylic acid residues)

IT **Peptides**, preparation
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(aminocycloalkanecarboxylic acid-contg., contrasting soln. conformations of **peptides** contg. .alpha.,.alpha.-dialkylglycine and aminocycloalkanecarboxylic acid residues)

IT 163493-04-7P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(contrasting soln. conformations of **peptides** contg. .alpha.,.alpha.-dialkylglycine and aminocycloalkanecarboxylic acid residues)

IT 163493-05-8P 163493-06-9P 163493-17-2P 163493-18-3P 163493-19-4P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(contrasting soln. conformations of **peptides** contg. .alpha.,.alpha.-dialkylglycine and aminocycloalkanecarboxylic acid residues)

IT 96-22-0, 3-Pentanone 108-94-1, Cyclohexanone, reactions 123-19-3, 4-Heptanone 502-42-1, Cycloheptanone 502-56-7, 5-Nonanone 2491-20-5, Alanine methyl ester hydrochloride 15761-38-3
RL: RCT (Reactant)
(contrasting soln. conformations of **peptides** contg. .alpha.,.alpha.-dialkylglycine and aminocycloalkanecarboxylic acid residues)

IT 702-62-5P, 1,3-Diazaspiro[4.5]decane-2,4-dione 707-16-4P, 1,3-Diazaspiro[4.6]undecane-2,4-dione 2566-29-2P, .alpha.,.alpha.-Diethylglycine 2566-31-6P, .alpha.,.alpha.-Dipropylglycine 2756-85-6P, 1-Aminocyclohexane-1-carboxylic acid 5455-34-5P, 5,5-Diethylhydantoin 6141-45-3P 6949-77-5P, 1-Aminocycloheptane-1-carboxylic acid 7148-46-1P, 2,4-Imidazolidinedione, 5,5-dibutyl- 7597-66-2P, .alpha.,.alpha.-Dibutylglycine 36033-33-7P 37993-32-1P 87113-23-3P 92398-50-0P 92398-54-4P 163493-07-0P 163493-08-1P 163493-09-2P 163493-10-5P 163493-11-6P 163493-12-7P 163493-13-8P 163493-14-9P 163493-15-0P 163493-16-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(contrasting soln. conformations of **peptides** contg. .alpha.,.alpha.-dialkylglycine and aminocycloalkanecarboxylic acid

residues)

=> fil reg

FILE 'REGISTRY' ENTERED AT 09:25:04 ON 05 SEP 2000
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

STRUCTURE FILE UPDATES: 4 SEP 2000 HIGHEST RN 288141-13-9
DICTIONARY FILE UPDATES: 4 SEP 2000 HIGHEST RN 288141-13-9

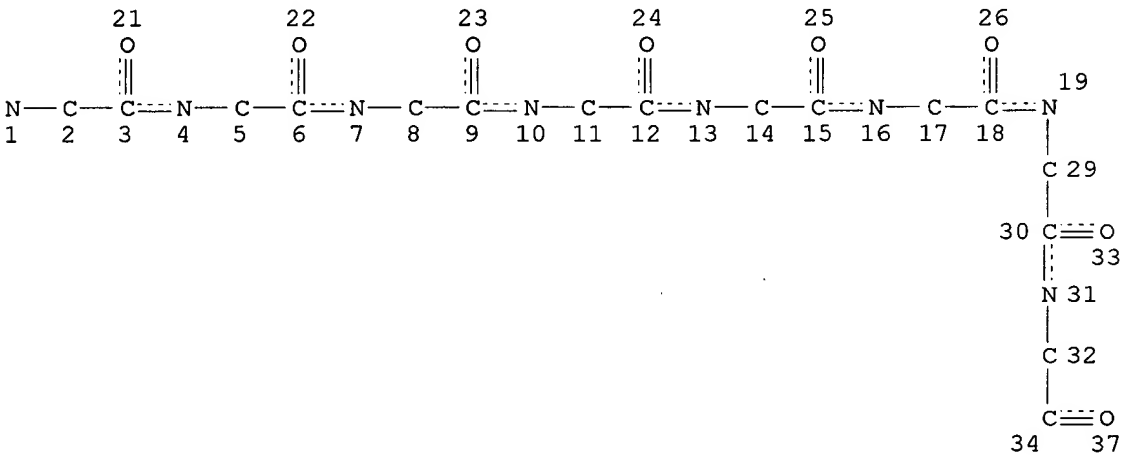
TSCA INFORMATION NOW CURRENT THROUGH JANUARY 11, 2000

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Structure search limits have been increased. See HELP SLIMIT for details.

=> d sta que l64

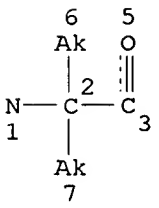
L28 27670 SEA FILE=REGISTRY ABB=ON PLU=ON PROTEIN/FS AND 8/SQL
L30 STR



NODE ATTRIBUTES:
NSPEC IS RC AT 2
NSPEC IS RC AT 5
NSPEC IS RC AT 8
NSPEC IS RC AT 11
NSPEC IS RC AT 14
NSPEC IS RC AT 17
NSPEC IS RC AT 29
NSPEC IS RC AT 32
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 32

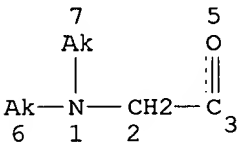
STEREO ATTRIBUTES: NONE
L32 10689 SEA FILE=REGISTRY SUB=L28 SSS FUL L30
L33 STR



NODE ATTRIBUTES:
CONNECT IS E1 RC AT 6
CONNECT IS E1 RC AT 7
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 6

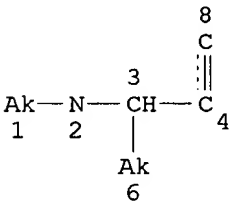
STEREO ATTRIBUTES: NONE
L34 STR



NODE ATTRIBUTES:
CONNECT IS E1 RC AT 6
CONNECT IS E1 RC AT 7
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 6

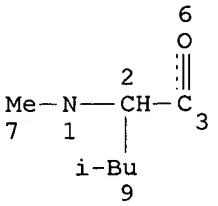
STEREO ATTRIBUTES: NONE
L35 STR



NODE ATTRIBUTES:
CONNECT IS E1 RC AT 1
CONNECT IS E1 RC AT 6
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 6

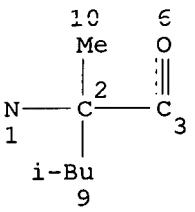
STEREO ATTRIBUTES: NONE
L36 STR



NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 6

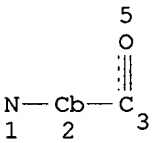
STEREO ATTRIBUTES: NONE
L37 STR



NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 6

STEREO ATTRIBUTES: NONE
L38 STR



NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 4

STEREO ATTRIBUTES: NONE

L40 244 SEA FILE=REGISTRY SUB=L32 SSS FUL (L33 OR L34 OR L35 OR L36 OR L37 OR L38)

L48 26 SEA FILE=REGISTRY ABB=ON PLU=ON (174350-44-8/BI OR 135013-53-5/BI OR 135013-54-6/BI OR 188064-10-0/BI OR 188064-21-3/BI OR 188064-25-7/BI OR 188064-27-9/BI OR 188064-28-0/BI OR 188064-30-4/BI OR 188064-32-6/BI OR 189098-41-7/BI OR 189098-42-8/BI OR 189098-43-9/BI OR 189098-44-0/BI OR 189098-45-1/BI OR 201984-90-9/BI OR 201984-94-3/BI OR 201984-95-4/BI OR 201984-99-8/BI OR 201985-00-4/BI OR 220331-94-2/BI OR 220332-02-5/BI OR 259107-45-4/BI OR 259107-49-8/BI OR 259107-50-1/BI OR 259107-54-5/BI)

L49 218 SEA FILE=REGISTRY ABB=ON PLU=ON L40 NOT L48

```
L50          10 SEA FILE=REGISTRY ABB=ON  PLU=ON  L49 AND (C3 OR C4 OR C5 OR
                C7 OR C8)/ES
L52           2 SEA FILE=REGISTRY ABB=ON  PLU=ON  L50 AND (C35H47N9O9 OR
                C50H88N8O11)
L53         186 SEA FILE=REGISTRY ABB=ON  PLU=ON  L49 NOT (NC4-C6 OR NCNC2)/ES

L54         184 SEA FILE=REGISTRY ABB=ON  PLU=ON  L53 NOT L50
L55         124 SEA FILE=REGISTRY ABB=ON  PLU=ON  L54 AND 46.150.18/RID
L56          60 SEA FILE=REGISTRY ABB=ON  PLU=ON  L54 NOT L55
L57          14 SEA FILE=REGISTRY ABB=ON  PLU=ON  L56 AND NR>=1
L58          46 SEA FILE=REGISTRY ABB=ON  PLU=ON  L56 NOT L57
L59           9 SEA FILE=REGISTRY ABB=ON  PLU=ON  L58 AND (C28H50N8O9 OR
                C29H52N8O9 OR C33H60N8O9 OR C32H62N8O9 OR C31H56N8O9 OR
                C34H62N8O9 OR C48H90N8O9 OR C32H58N8O9 OR C49H92N8O9)
L64          11 SEA FILE=REGISTRY ABB=ON  PLU=ON  (L52 OR L59)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L64  ANSWER 1 OF 11  REGISTRY  COPYRIGHT 2000 ACS
RN   281664-71-9  REGISTRY
CN   Alanine, 2-methylalanyl-2-methylalanyl-L-leucyl-2-methylalanyl-2-
     methylalanyl-2-methylalanyl-2-methylalanyl-2-methyl- (9CI)  (CA INDEX
     NAME)
FS   PROTEIN SEQUENCE; STEREOSEARCH
SQL  8
NTE
```

type	------ location ------		description
uncommon	Aib-1	-	-
uncommon	Aib-2	-	-
uncommon	Aib-4	-	-
uncommon	Aib-5	-	-
uncommon	Aib-6	-	-
uncommon	Aib-7	-	-
uncommon	Aib-8	-	-

```
SEQ      1 XXLXXXXX
MF   C34 H62 N8 O9
SR   CA
LC   STN Files:   CA, CAPLUS

Absolute stereochemistry.
```

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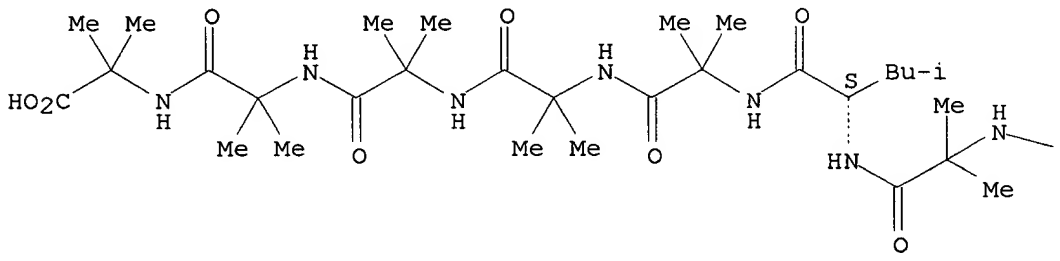
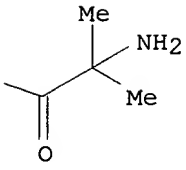


PAGE 1-B



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 133:89770

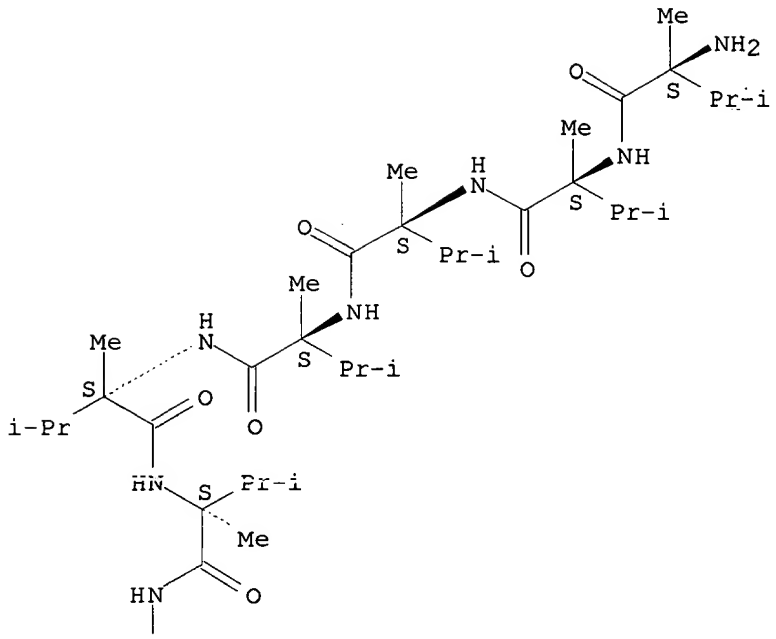
L64 ANSWER 2 OF 11 REGISTRY COPYRIGHT 2000 ACS
RN 281664-70-8 REGISTRY
CN L-Isovaline, 3-methyl-L-isovalyl-3-methyl-L-isovalyl-3-methyl-L-isovalyl-3-methyl-L-isovalyl-3-methyl-L-isovalyl-3-methyl-L-isovalyl-3-methyl-L-isovalyl-3-methyl- (9CI) (CA INDEX NAME)
FS PROTEIN SEQUENCE; STEREOSEARCH
SQL 8
NTE modified

type	------ location ------		description
modification	Val-1	-	undetermined modification
modification	Val-2	-	undetermined modification
modification	Val-3	-	undetermined modification
modification	Val-4	-	undetermined modification
modification	Val-5	-	undetermined modification
modification	Val-6	-	undetermined modification
modification	Val-7	-	undetermined modification
modification	Val-8	-	undetermined modification

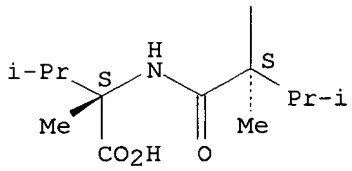
SEQ 1 VVVVVVVV
MF **C48 H90 N8 O9**
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 133:89770

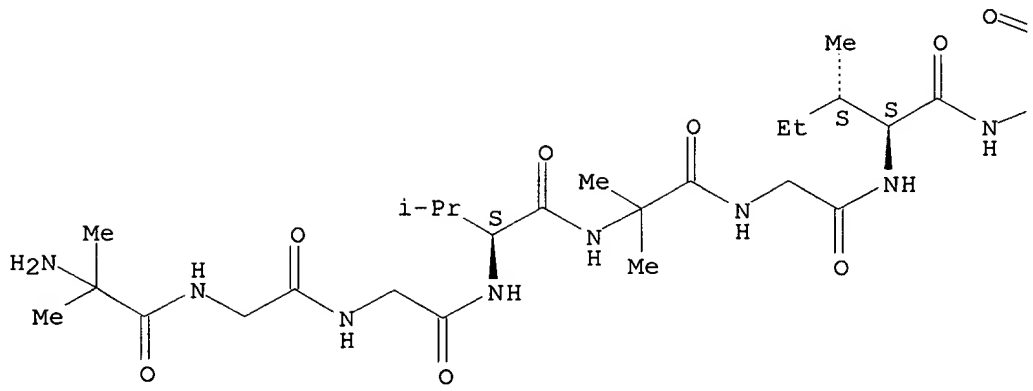
L64 ANSWER 3 OF 11 REGISTRY COPYRIGHT 2000 ACS
RN 223617-32-1 REGISTRY
CN 4-10-Trikoningin KB I, 10-L-isoleucine-10a-L-leucine-, methyl ester (9CI) (CA INDEX NAME)
FS PROTEIN SEQUENCE; STEREOSEARCH
SQL 8
NTE modified

type	------ location ------		description
uncommon	Aib-1	-	-
uncommon	Aib-5	-	-

SEQ 1 XGGVXGIL
MF **C32 H58 N8 O9**
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

PAGE 1-A



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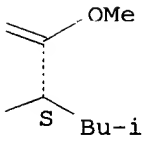


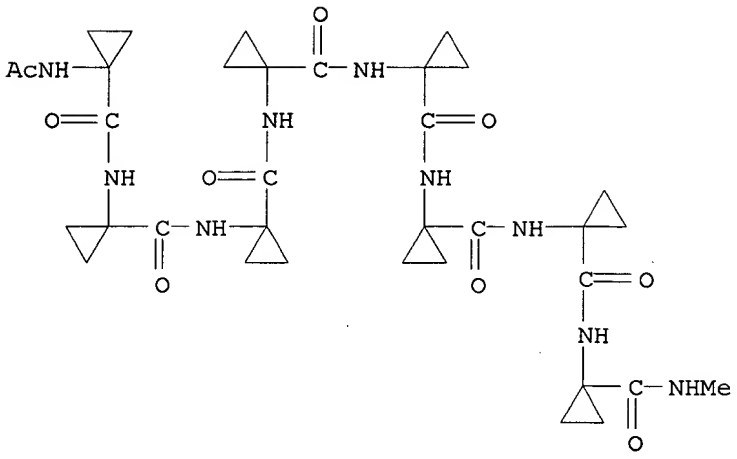
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 130:312066

L64 ANSWER 4 OF 11 REGISTRY COPYRIGHT 2000 ACS
RN 214058-85-2 REGISTRY
CN Cyclopropanecarboxamide, 1-[[[1-[[[1-[[[1-[[[1-(acetylamino)cyclopropyl]carbonyl]amino]cyclopropyl]carbonyl]amino]cyclopropyl]carbonyl]amino]cyclopropyl]carbonyl]amino]-N-[1-[[[1-[[[1-[(methylamino)carbonyl]cyclopropyl]amino]carbonyl]cyclopropyl]amino]carbonyl]cyclopropyl]- (9CI) (CA INDEX NAME)
FS PROTEIN SEQUENCE
SQL 8
NTE modified (modifications unspecified)

type	location		description
uncommon	Aaa-1	-	-
uncommon	Aaa-2	-	-
uncommon	Aaa-3	-	-
uncommon	Aaa-4	-	-
uncommon	Aaa-5	-	-
uncommon	Aaa-6	-	-
uncommon	Aaa-7	-	-
uncommon	Aaa-8	-	-

SEQ 1 XXXXXXXX
MF **C35 H47 N9 O9**
SR CA
LC STN Files: CA, CAPLUS



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:276333

L64 ANSWER 5 OF 11 REGISTRY COPYRIGHT 2000 ACS
RN 183667-57-4 REGISTRY
CN L-Valine, N-[(1,1-dimethylethoxy)carbonyl]-L-leucyl-1-aminocyclooctanecarbonyl-L-valylglycylglycyl-L-leucyl-1-aminocyclooctanecarbonyl-, methyl ester (9CI) (CA INDEX NAME)
FS PROTEIN SEQUENCE; STEREOSEARCH
SQL 8
NTE modified (modifications unspecified)

type	------ location ------		description
uncommon	Aaa-2	-	-
uncommon	Aaa-7	-	-

SEQ 1 LXVGGLXV
MF **C50 H88 N8 O11**
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

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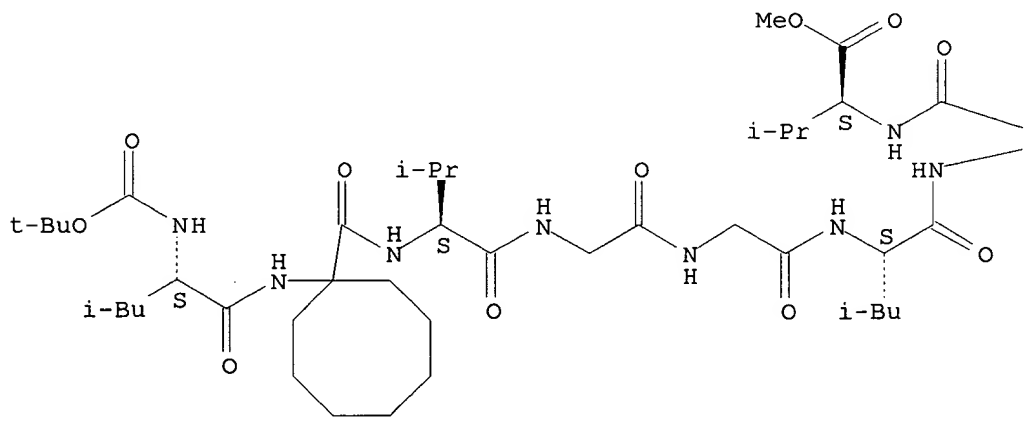

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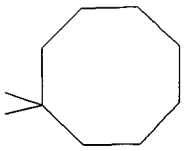

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 125:320867

L64 ANSWER 6 OF 11 REGISTRY COPYRIGHT 2000 ACS
RN 176664-81-6 REGISTRY
CN 4-10-Trichogin A IV, 9-L-isoleucine-10a-L-leucine-, methyl ester (9CI) (CA INDEX NAME)
FS PROTEIN SEQUENCE; STEREOSEARCH
SQL 8
NTE modified

type	------ location ------		description
uncommon	Aib-1	-	-
uncommon	Aib-5	-	-

SEQ 1 XGGLXGIL
MF **C33 H60 N8 O9**
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

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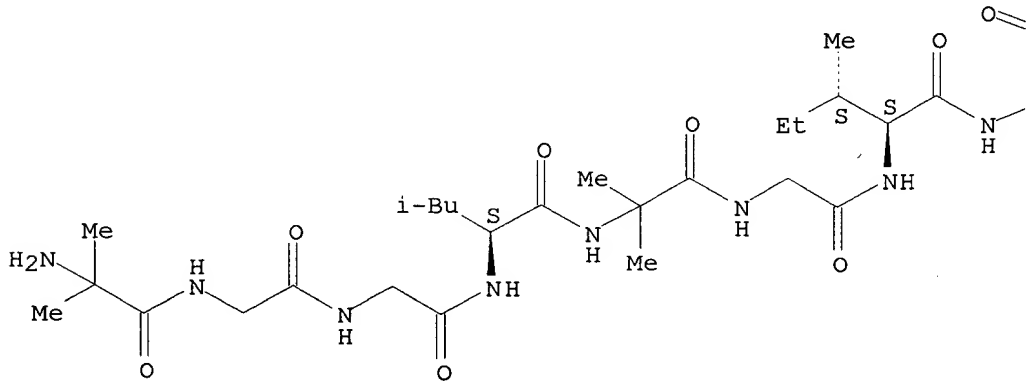

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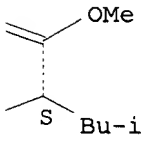

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 124:336177

L64 ANSWER 7 OF 11 REGISTRY COPYRIGHT 2000 ACS
RN 148505-60-6 REGISTRY
CN Alanine, N-[N-[N-[N-[N-(N-L-alanyl-2-methylalanyl)-L-alanyl]-2-methylalanyl]-L-alanyl]-2-methylalanyl]-L-alanyl]-2-methyl-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)
FS PROTEIN SEQUENCE; STEREOSEARCH
SQL 8
NTE modified

type	------ location ------		description
uncommon	Aib-2	-	-
uncommon	Aib-4	-	-
uncommon	Aib-6	-	-
uncommon	Aib-8	-	-
modification	-	-	undetermined modification

SEQ 1 AXAXAXAX
MF **C29 H52 N8 O9 . Cl H**
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

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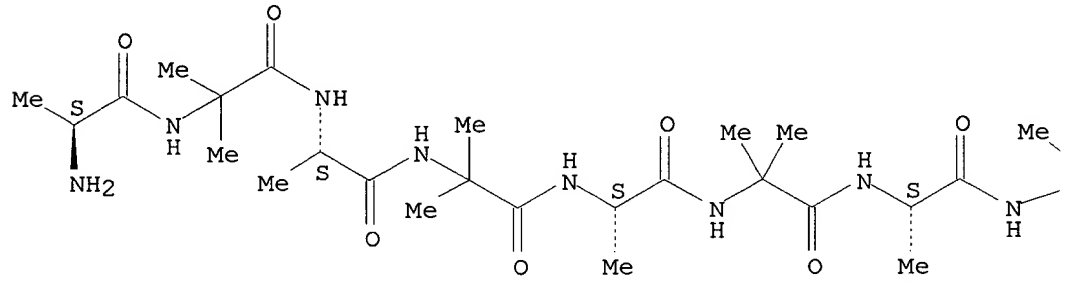

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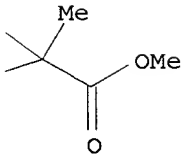

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 119:43723

L64 ANSWER 8 OF 11 REGISTRY COPYRIGHT 2000 ACS
RN 143868-51-3 REGISTRY
CN Alanine, 2-methyl-N-[N-[2-methyl-N-[N-[2-methyl-N-[N-(N-L-valylglycyl)-L-alanyl]alanyl]-L-alanyl]alanyl]-L-valyl]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)
FS PROTEIN SEQUENCE
SQL 8
NTE modified

type	------ location ------		description
uncommon	Aib-4	-	-
uncommon	Aib-6	-	-
uncommon	Aib-8	-	-
modification	-	-	undetermined modification

SEQ 1 VGAXAXVX
MF **C31 H56 N8 O9 . Cl H**
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

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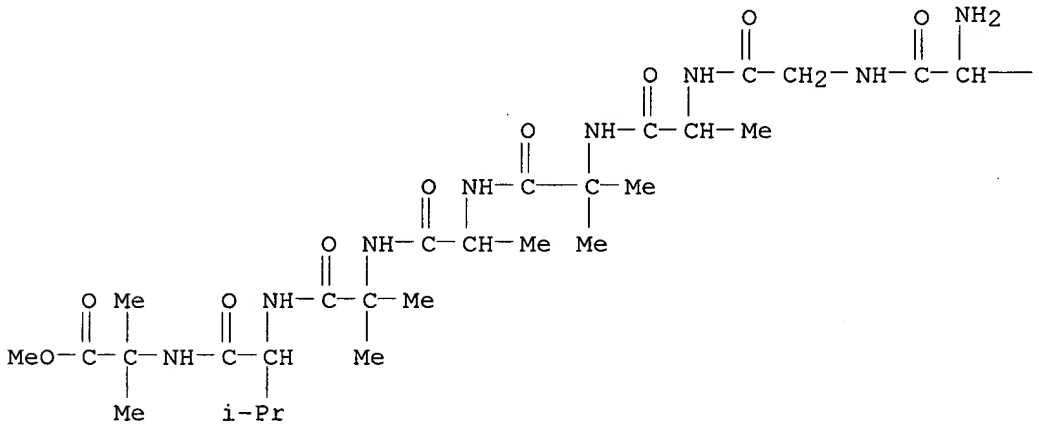

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1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 117:172078

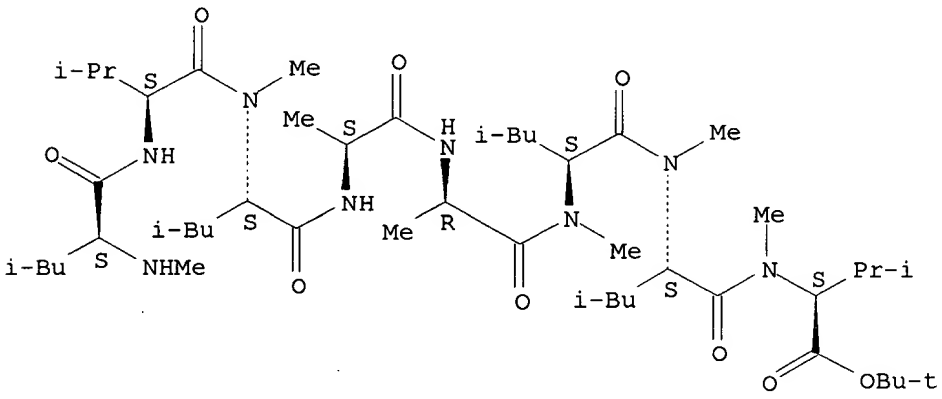
L64 ANSWER 9 OF 11 REGISTRY COPYRIGHT 2000 ACS
RN 117106-24-8 REGISTRY
CN L-Valine, N-methyl-N-[N-methyl-N-[N-methyl-N-[N-[N-[N-methyl-N-[N-(N-methyl-L-leucyl)-L-valyl]-L-leucyl]-L-alanyl]-D-alanyl]-L-leucyl]-L-leucyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)
FS PROTEIN SEQUENCE; STEREOSEARCH

SQL 8
NTE modified

type	------ location ------		description
modification	Leu-1	-	methyl<Me>
modification	Leu-3	-	methyl<Me>
modification	Leu-6	-	methyl<Me>
modification	Leu-7	-	methyl<Me>
modification	Val-8	-	methyl<Me>

SEQ 1 LVLAALLV
MF **C49 H92 N8 O9**
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
(*File contains numerically searchable property data)

Absolute stereochemistry.



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 109:190816

L64 ANSWER 10 OF 11 REGISTRY COPYRIGHT 2000 ACS
RN 100843-78-5 REGISTRY
CN Alanine, 2-methyl-N-[2-methyl-N-[N-[N-[N-[2-methyl-N-[2-methyl-N-(2-methylalanyl)alanyl]alanyl]-L-valyl]glycyl]-L-leucyl]alanyl]-, methyl ester (9CI) (CA INDEX NAME)
FS PROTEIN SEQUENCE; STEREOSEARCH
SQL 8
NTE modified

type	------ location ------		description
uncommon	Aib-1	-	-
uncommon	Aib-2	-	-
uncommon	Aib-3	-	-
uncommon	Aib-7	-	-
uncommon	Aib-8	-	-

SEQ 1 XXXVGLXX
MF **C34 H62 N8 O9**
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

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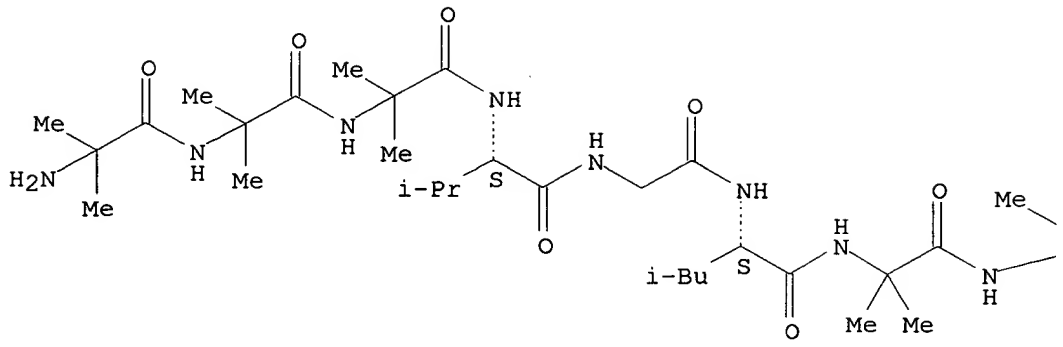
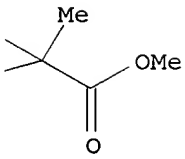


PAGE 1-B



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 104:104617

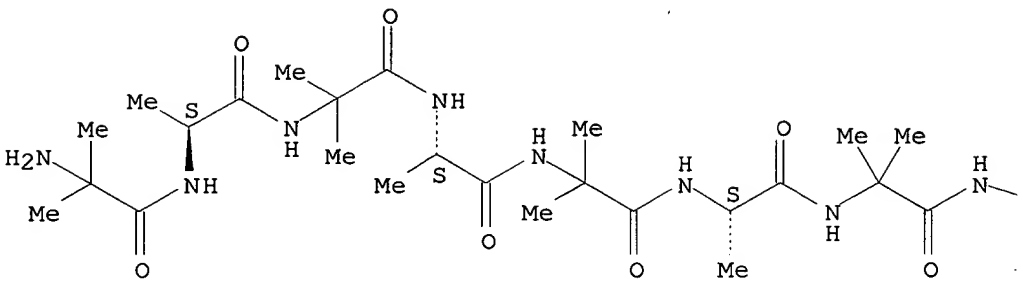
L64 ANSWER 11 OF 11 REGISTRY COPYRIGHT 2000 ACS
RN 70134-43-9 REGISTRY
CN L-Alanine, N-[2-methyl-N-[N-[2-methyl-N-[N-[2-methyl-N-[N-(2-methylalanyl)-L-alanyl]alanyl]-L-alanyl]alanyl]-L-alanyl]alanyl]- (9CI) (CA INDEX NAME)
FS PROTEIN SEQUENCE; STEREOSEARCH
SQL 8
NTE

type	location		description
uncommon	Aib-1	-	-
uncommon	Aib-3	-	-
uncommon	Aib-5	-	-
uncommon	Aib-7	-	-

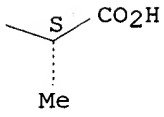
SEQ 1 XAXAXAXA
MF **C28 H50 N8 O9**
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 90:187312

=> d his l64-

(FILE 'REGISTRY' ENTERED AT 08:54:10 ON 05 SEP 2000)
L64 11 S L52,L59
SAV L64 MOEZIE248B/A

FILE 'HCAOLD' ENTERED AT 09:24:50 ON 05 SEP 2000
L65 0 S L64

FILE 'HCAPLUS' ENTERED AT 09:24:57 ON 05 SEP 2000
L66 10 S L64

FILE 'REGISTRY' ENTERED AT 09:25:04 ON 05 SEP 2000

=> fil hcaplus

FILE 'HCAPLUS' ENTERED AT 09:25:19 ON 05 SEP 2000

FILE COVERS 1967 - 5 Sep 2000 VOL 133 ISS 11
FILE LAST UPDATED: 4 Sep 2000 (20000904/ED)

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=> d all tot l66

L66 ANSWER 1 OF 10 HCAPLUS COPYRIGHT 2000 ACS
AN 2000:211479 HCAPLUS
DN 133:89770
TI Simulations of oligopeptide vibrational CD: effects of isotopic labeling
AU Bour, Petr; Kubelka, Jan; Keiderling, Timothy A.
CS Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Prague, 16610/6, Czech Rep.
SO Biopolymers (2000), 53(5), 380-395
CODEN: BIPMAA; ISSN: 0006-3525
PB John Wiley & Sons, Inc.
DT Journal
LA English
CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 22
AB Simulated IR absorption and vibrational CD (VCD) spectra of alanine-based octapeptides, each having its main chain constrained to a different secondary structure conformation (.alpha.-helix, 310-helix, ProII-like helix and .beta.-sheet-like strand), were analyzed and compared with exptl. results for several different peptides. The octapeptide simulations were based on transfer of property tensors from a series of ab initio calcns. for a short L-alanine based segment contg. 3 peptide bonds with relative .phi., .psi. angles fixed to those appropriate for .alpha.-helix, 310-helix, ProII-like helix, and .beta.-sheet-like strand. The tripeptide force field (FF) and at. polar tensors were obtained with d. functional theory techniques at the BPW91/6-31G** level and the at. axial tensor at the mixed BPW91/6-31G**/HF/6-31G level. Allowing for frequency correction due to the FF limitations, the octapeptide results obtained are qual. consistent with exptl. observations for IR and VCD spectra of polypeptides and oligopeptides in established conformations. In all cases, the correct VCD sign patterns for the amide I and II bands were predicted, but the intensities did have some variation from the exptl. patterns. Predicted VCD changes upon deuteration of either the peptide or side-chains as well as for 13C isotopic labeling of the amide C:O at specific sites in the peptide chain were computed for anal. of exptl. observations. A combination of theor. modeling with exptl. data for labeled compds. leads both to enhanced resoln. of component transitions and added conformational applicability of the VCD spectra.
ST alanine octapeptide vibrational CD simulation isotope labeling effect; secondary structure conformation simulated alanine octapeptide
IT Helix (conformation)
(310-helical; calcd. conformational data and simulated vibrational CD spectra for the model alanine octapeptide)
IT Immunoglobulins
RL: PRP (Properties)
(G; exptl. vibrational CD data for comparing with the computed vibrational CD of model alanine octapeptide)
IT Ab initio methods
Conformation
Simulation and Modeling, physicochemical
.alpha.-Helix
.beta.-Sheet

(calcd. conformational data and simulated vibrational CD spectra for the model alanine octapeptide)
IT Isotope effect
Secondary structure
Vibrational circular dichroism
(effect of isotopic labeling on simulated vibrational CD spectra for the model alanine octapeptide)
IT Peptides, properties
RL: PRP (Properties)
(oligopeptides; calcd. conformational data and simulated vibrational CD spectra for the model alanine octapeptide)
IT Conformation
(.beta.-turn, type II; effect of isotopic labeling on simulated vibrational CD spectra for the model alanine octapeptide)
IT 128371-85-7
RL: PRP (Properties)
(calcd. conformational data and simulated vibrational CD spectra for the model alanine octapeptide)
IT 281664-72-0 281664-73-1 281664-74-2 281664-75-3
RL: PRP (Properties)
(effect of isotopic labeling on simulated vibrational CD spectra for the model alanine octapeptide)
IT 21379-66-8 25014-27-1, Poly-.gamma.-benzyl-L-Glutamate 25038-53-3
25104-18-1, Poly(L-lysine) 38000-06-5, Poly(L-lysine), SRU 64809-02-5
64809-10-5 281664-68-4 **281664-70-8 281664-71-9**
RL: PRP (Properties)
(exptl. vibrational CD data for comparing with the computed vibrational CD of model alanine octapeptide)
IT 27482-45-7
RL: PRP (Properties)
(simulated vibrational CD spectra for the model pseudo-alanine-tripeptide)
RE.CNT 98
RE
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L66 ANSWER 2 OF 10 HCAPLUS COPYRIGHT 2000 ACS
AN 1999:187356 HCAPLUS
DN 130:312066
TI Total synthesis and membrane modifying properties of the lipopeptaibol Trikoningin KB II and its analogs with acyl chains of different length at the N- and C-termini
AU Piazza, Claudia; Formaggio, Fernando; Crisma, Marco; Toniolo, Claudio; Kamphuis, Johan; Kaptein, Bernard; Broxterman, Quirinus B.
CS Department of Organic Chemistry, Biopolymer Research Centre, C.N.R., University of Padova, Padua, 35131, Italy
SO J. Pept. Sci. (1999), 5(2), 96-102
CODEN: JPSIEI; ISSN: 1075-2617
PB John Wiley & Sons Ltd.
DT Journal
LA English
CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 1
AB Trikoningin KB II, a ten-amino acid residue lipopeptaibol blocked at the N-terminus by the n-octanoyl group and at the C-terminus by the 1,2-amino alc. L-leucinol, and extd. from the fungus Trichoderma koningii, exhibits membrane-modifying properties. The authors have synthesized by soln.-phase methods trikoningin KB II and several analogs with acyl chains of different length at the N- and C-termini. Lipopeptaibols bind to phospholipid bilayers and are able to modify their permeability. Therefore, the permeability properties of trikoningin KB II and its analogs with acyl chains of different length at the N- and C-termini were investigated by following fluorimetrically the induced CF leakage from small unilamellar vesicles (egg PC-cholesterol 70:30) for different Rt-1 = [peptide]/[lipid] molar ratios. Permeability measurements showed that an appropriate length of the linear acyl chain is a more important characteristic for the onset of significant membrane-modifying activity than its position in the peptide chain. New relevant information extd. from this work may be summarized as follows: (i) in striking contrast to the effect produced by one long (C8) acyl chain, two short (C4) acyl chains, each with half no. of carbon atoms, concomitantly linked at the two termini of the peptide chain, are not able to induce any appreciable membrane activity; (ii) the position of the long acyl chain does have some influence, albeit not dramatic, on membrane activity (it is higher when the C8 acyl chain is located at the N-terminus of the peptide chain); (iii) the presence of two C8 acyl chains, concomitantly linked at the two termini of the peptide chain, produces a significant increase in membrane activity.
ST lipopeptaibol trikoningin KB II analog prepn membrane modifying activity; peptide prepn acyl chain length membrane; permeability membrane trikoningin KB II analog
IT Cell membrane
Membranes (biological)
Permeability
(total synthesis and membrane modifying properties of lipopeptaibol Trikoningin KB II and its analogs with acyl chains of different length at N- and C-termini)
IT Peptides, preparation
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(total synthesis and membrane modifying properties of lipopeptaibol Trikoningin KB II and its analogs with acyl chains of different length at N- and C-termini)
IT 223616-71-5P 223616-75-9P 223616-77-1P 223616-79-3P 223616-82-8P
223616-86-2P 223616-90-8P 223616-92-0P 223616-94-2P
RL: BUU (Biological use, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(total synthesis and membrane modifying properties of lipopeptaibol Trikoningin KB II and its analogs with acyl chains of different length at N- and C-termini)

IT 1138-80-3 1149-26-4 2666-93-5 3160-59-6 15030-72-5 163312-63-8, Z-D-Iva-OH
RL: RCT (Reactant)
(total synthesis and membrane modifying properties of lipopeptaibol Trikoningin KB II and its analogs with acyl chains of different length at N- and C-termini)

IT 4818-03-5P 15030-74-7P, (Z-Aib)2O 54793-59-8P 119768-28-4P
156916-67-5P 164575-77-3P 176664-73-6P 223616-46-4P 223616-49-7P
223616-53-3P 223616-57-7P 223616-61-3P 223616-65-7P 223616-67-9P
223617-15-0P 223617-22-9P 223617-28-5P **223617-32-1P**
223617-35-4P 223617-38-7P 223617-42-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(total synthesis and membrane modifying properties of lipopeptaibol Trikoningin KB II and its analogs with acyl chains of different length at N- and C-termini)

RE.CNT 30
RE
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L66 ANSWER 3 OF 10 HCAPLUS COPYRIGHT 2000 ACS
AN 1998:590250 HCAPLUS
DN 129:276333
TI PAPQMD parametrization of molecular systems with cyclopropyl rings: conformational study of homopeptides constituted by 1-aminocyclopropane-1-carboxylic acid
AU Aleman, Carlos; Casanovas, Jordi; Galembeck, Sergio E.
CS Departament d'Enginyeria Quimica, Universitat Politecnica de Catalunya, Barcelona, E-08028, Spain
SO J. Comput.-Aided Mol. Des. (1998), 12(3), 259-273
CODEN: JCADEQ; ISSN: 0920-654X
PB Kluwer Academic Publishers
DT Journal
LA English
CC 34-3 (Amino Acids, Peptides, and Proteins)

Section cross-reference(s): 22

AB The suitability of ab initio, semiempirical and d. functional methods as sources of stretching and bending parameters has been explored using the PAPQMD (program for approx. parametrization from quantum mech. data) strategy. Results show that semiempirical methods provide parameters comparable to those compiled on empirical force fields. In this respect the AM1 method seems to be a good method to obtain parameters at a min. computational cost. On the other hand, harmonic force fields initially developed for proteins and DNA have been extended to include compds. contg. highly strained three-membered rings, like 1-aminocyclopropane-1-carboxylic acid. For this purpose the cyclopropyl ring has been explicitly parametrized at the AM1 level considering different chem. environments. Finally, the new set of parameters has been used to investigate the conformational preferences of homopeptides constituted by 1-aminocyclopropane-1-carboxylic acid. Results indicate that such compds. tend to adopt a helical conformation stabilized by intramol. hydrogen bonds between residues i and i + 3. This conformation allows the arrangement of the cyclic side chains without steric clashes.

ST aminocyclopropanecarboxylic acid homopeptide conformation PAPQMD parametrization; AM1 MO aminocyclopropanecarboxylic acid homopeptide conformation

IT AM1 MO (molecular orbital)
Conformation
(PAPQMD parametrization of mol. systems with cyclopropyl rings and conformational study of aminocyclopropanecarboxylic acid homopeptides)

IT Peptides, properties
RL: PRP (Properties)
(aminocyclopropanecarboxylic acid-contg.; PAPQMD parametrization of mol. systems with cyclopropyl rings and conformational study of aminocyclopropanecarboxylic acid homopeptides)

IT 75-19-4, Cyclopropane 22059-21-8, 1-Aminocyclopropane-1-carboxylic acid 99451-23-7 126705-26-8 129618-40-2, Nevirapine 214058-82-9 214058-83-0 **214058-85-2** 214058-86-3 214058-87-4
RL: PRP (Properties)
(PAPQMD parametrization of mol. systems with cyclopropyl rings and conformational study of aminocyclopropanecarboxylic acid homopeptides)

L66 ANSWER 4 OF 10 HCAPLUS COPYRIGHT 2000 ACS
AN 1996:701427 HCAPLUS
DN 125:320867
TI NMR analysis of a conformational transition in an acyclic peptide. Model system for studying helix unfolding
AU Raghothama, S.; Chaddha, M.; Balaram, P.
CS Molecular Biophysics Unit, Indian Institute of Science, Bangalore, 560 012, India
SO J. Phys. Chem. (1996), 100(50), 19666-19671
CODEN: JPCHAX; ISSN: 0022-3654
DT Journal
LA English
CC 6-3 (General Biochemistry)
Section cross-reference(s): 34

AB The stabilization of helical structures in short apolar peptides is readily achieved by introduction of .alpha.,.alpha.-dialkylamino acids. The use of stereochem. constrained residues in conjunction with conformationally flexible segments permits the design of peptides that are poised to undergo structural transitions. The octapeptide Boc-Leu-Ac8c-Val-Gly-Gly-Leu-Ac8c-Val-OMe (Ac8c = 1-aminocyclooctane-1-carboxylic acid) incorporates residues with contradictory conformational tendencies. NMR anal. in CDCl3, using nuclear Overhauser effects and delineation of hydrogen-bonded NH groups establishes a 310-helical conformation. In a polar strongly solvating medium, like DMSO, the helix unfolds. Studies in CDCl3/DMSO mixts. provide clear evidence for a solvent dependent conformational transition. Amide NH chem. shifts and temp. coeffs. at varying solvent compn. allow a detailed structural anal. of the unfolding process. The intrinsic fragility of the octapeptide helix provides an opportunity to examine invasion of the helix backbone by

water mols. Studies in DMSO soln. contg. low concns. of water establish that preferential water peptide interactions may indeed be present.
ST helix unfolding NMR model acyclic octapeptide
IT Hydrogen bond
Nuclear magnetic resonance
Overhauser effect
Simulation and Modeling, biological
(NMR anal. of conformational transition in acyclic peptide Boc-Leu-Ac8c-Val-Gly-Gly-Leu-Ac8c-Val-OMe as model system for studying helix unfolding)
IT Peptides, properties
RL: PRP (Properties)
(helix unfolding; NMR anal. of conformational transition in acyclic peptide Boc-Leu-Ac8c-Val-Gly-Gly-Leu-Ac8c-Val-OMe as model system for studying helix unfolding)
IT Conformation and Conformers
(helical, NMR anal. of conformational transition in acyclic peptide Boc-Leu-Ac8c-Val-Gly-Gly-Leu-Ac8c-Val-OMe as model system for studying helix unfolding)
IT **183667-57-4**
RL: PRP (Properties)
(Boc-Leu-Ac8c-Val-Gly-Gly-Leu-Ac8c-Val-OMe; NMR anal. of conformational transition in acyclic peptide Boc-Leu-Ac8c-Val-Gly-Gly-Leu-Ac8c-Val-OMe as model system for studying helix unfolding)
IT 67-68-5, DMSO, biological studies 865-49-6
RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)
(NMR anal. of conformational transition in acyclic peptide Boc-Leu-Ac8c-Val-Gly-Gly-Leu-Ac8c-Val-OMe as model system for studying helix unfolding)

L66 ANSWER 5 OF 10 HCAPLUS COPYRIGHT 2000 ACS
AN 1996:288176 HCAPLUS
DN 124:336177
TI Effect of N.alpha.-Acyl Chain Length on the Membrane-Modifying Properties of Synthetic Analogs of the Lipopeptaibol Trichogin GA IV
AU Toniolo, C.; Crisma, M.; Formaggio, F.; Peggion, C.; Monaco, V.; Goulard, C.; Rebuffat, S.; Bodo, B.
CS Department of Organic Chemistry, University of Padova, Padua, 35131, Italy
SO J. Am. Chem. Soc. (1996), 118(21), 4952-4958
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA English
CC 6-6 (General Biochemistry)
Section cross-reference(s): 34
AB Trichogin GA IV, an 11-residue lipopeptaibol blocked at the N-terminus by an n-octanoyl group and at the C-terminus by a 1,2-amino alc. (L-leucinol), extd. from the fungus Trichoderma longibrachiatum, exhibits remarkable membrane-modifying properties. We have synthesized trichogin GA IV and several [L-Leu-OMe11] analogs carrying at the N-terminus an acyl chain of variable length (C2-C8, C10, C12, C14, C16, C18). A succinylated head-to-head dimer was also prepd. A conformational anal., carried out by FTIR absorption, CD, and NMR, showed that the right-handed helical structure of the natural lipopeptaibol is essentially preserved in all its analogs. Permeability measurements revealed that at least six carbon atoms in the N.alpha.-blocking fatty acyl moiety are required for the onset of significant membrane-modifying properties. Also the head-to-head dimer is remarkably active. Possible models for the mechanism of membrane permeability of trichogin GA IV are discussed.
ST lipopeptaibol trichogin GA IV membrane permeability; lipopeptide trichogin analog prepn membrane permeability
IT Antibiotics
Conformation and Conformers
(synthesis of lipopeptaibol trichogin GA IV and analogs and effect of N.alpha.-acyl chain length on membrane-modifying properties and antibacterial activity)

IT Lipopeptides
RL: BAC (Biological activity or effector, except adverse); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis of lipopeptaibol trichogin GA IV and analogs and effect of N.alpha.-acyl chain length on membrane-modifying properties and antibacterial activity)
IT Molecular structure-biological activity relationship
(membrane permeability-affecting, synthesis of lipopeptaibol trichogin GA IV and analogs and effect of N.alpha.-acyl chain length on membrane-modifying properties and antibacterial activity)
IT Biological transport
(permeation, synthesis of lipopeptaibol trichogin GA IV and analogs and effect of N.alpha.-acyl chain length on membrane-modifying properties and antibacterial activity)
IT 138531-93-8P, Trichogin GA IV 173739-68-9P 176664-85-0P 176664-86-1P
176664-87-2P 176664-88-3P 176664-89-4P 176664-90-7P 176664-91-8P
176664-92-9P 176664-93-0P 176664-94-1P 176664-95-2P 176664-96-3P
RL: BAC (Biological activity or effector, except adverse); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis of lipopeptaibol trichogin GA IV and analogs and effect of N.alpha.-acyl chain length on membrane-modifying properties and antibacterial activity)
IT 99176-53-1 106897-28-3 106897-29-4 125615-20-5 141745-54-2
176664-97-4 176664-98-5 176664-99-6 176665-00-2 176665-01-3
176665-02-4 176665-03-5 176665-04-6 176665-05-7 176665-06-8
176665-07-9 176665-08-0 176665-09-1 176665-10-4 176665-11-5
RL: PRP (Properties); RCT (Reactant)
(synthesis of lipopeptaibol trichogin GA IV and analogs and effect of N.alpha.-acyl chain length on membrane-modifying properties and antibacterial activity)
IT 543-20-4, Butanedioyl dichloride 1212-53-9 2018-66-8 2666-93-5
3160-59-6 4818-03-5 15030-72-5 15030-74-7 54793-59-8 176664-71-4
176664-72-5 176665-12-6
RL: RCT (Reactant)
(synthesis of lipopeptaibol trichogin GA IV and analogs and effect of N.alpha.-acyl chain length on membrane-modifying properties and antibacterial activity)
IT 119768-28-4P 156916-67-5P 164575-77-3P 173739-67-8P 173739-69-0P
176664-73-6P 176664-74-7P 176664-75-8P 176664-76-9P 176664-77-0P
176664-78-1P 176664-79-2P 176664-80-5P **176664-81-6P**
176664-82-7P 176664-83-8P 176664-84-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(synthesis of lipopeptaibol trichogin GA IV and analogs and effect of N.alpha.-acyl chain length on membrane-modifying properties and antibacterial activity)

L66 ANSWER 6 OF 10 HCAPLUS COPYRIGHT 2000 ACS
AN 1993:443723 HCAPLUS
DN 119:43723
TI Orientation change of glycopeptide in lipid bilayer membrane induced by lectin binding
AU Otoda, Kazuya; Kimura, Shunsaku; Imanishi, Yukio
CS Dep. Polym. Chem., Kyoto Univ., Yoshida Honmachi, Sakyo-ku, Kyoto, Japan
SO Biochim. Biophys. Acta (1993), 1145(1), 33-41
CODEN: BBACAQ; ISSN: 0006-3002
DT Journal
LA English
CC 6-6 (General Biochemistry)
AB A lectin-induced orientation change of a helical glycopeptide in lipid bilayer membranes was studied. Glycopeptides composed of hydrophobic nona-(G8) and pentapeptide (G4) with a fluorescent probe at the N-terminal and a lactose unit at the C-terminal were synthesized. The glycopeptides were incorporated into lipid bilayer membranes (BLM) with the lactose unit exposed to the aq. phase and the peptide chain buried in the membrane. G8

takes a partially helical structure in the membrane, while G4 an irregular structure. Upon binding of lectin to G8 held in the membrane of dipalmitoylphosphatidylcholine (DPPC) liposome, enhancement of fluorescence intensity of the N-terminal anthryl group, redn. of fluorescence quenching of the anthryl group with acrylamide, and increase of CF-leakage from the DPPC liposome were obsd. G8', which lacks the O-anthrylmethylserine residue from G8, formed a voltage-dependent ion channel in BLM expts. The frequency of single current fluctuations induced by G8' incorporation increased with addn. of lectin. These results indicate that the peptide segment of G8 prefers taking a more perpendicular orientation to the membrane upon assocn. with lectin.

ST glycopeptide helix phosphatidylcholine bilayer orientation lectin; agglutinin RCA60 glycopeptide membrane orientation; ion channel glycopeptide bilayer membrane

IT Agglutinins and Lectins
RL: BIOL (Biological study)
(RCA60, helical glycopeptide orientation in phosphatidylcholine bilayer membrane response to)

IT Phosphatidylcholines, biological studies
RL: BIOL (Biological study)
(bilayer membrane, glycopeptide orientation in, lectin effect on)

IT Ion channel
(formation of voltage-dependent, by glycopeptide and hydrophobic helical peptide in phospholipid planar bilayer)

IT Molecular orientation
(of helical glycopeptide, in phosphatidylcholine bilayer membrane, lectin effect on)

IT Glycopeptides
RL: PRP (Properties)
(orientation of, in phosphatidylcholine bilayer membrane, lectin effect on)

IT Membrane, biological
(bilayer, phosphatidylcholine, glycopeptide orientation in, lectin effect on)

IT Electric activity
(current-potential relationship, of glycopeptide and hydrophobic helical peptide ion channel in phospholipid planar bilayer)

IT Conformation and Conformers
(.alpha.-helical, of glycononapeptide in phosphatidylcholine bilayer membrane)

IT 2644-64-6, Dipalmitoylphosphatidylcholine 13699-48-4, Dimyristoylphosphatidylcholine
RL: BIOL (Biological study)
(bilayer membrane, glycopeptide orientation in, lectin effect on)

IT 148505-61-7P 148505-62-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and conformation and orientation in phosphatidylcholine bilayer membrane of, lectin effect on)

IT 74426-35-0P 148505-59-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and coupling with peptide derivs. of)

IT **148505-60-6P** 148526-29-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and coupling with serine derivs. of)

IT 148526-30-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and hydrogenation of)

IT 148505-63-9P 148505-64-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and hydroxylation of)

IT 136198-08-8P 148505-65-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and ion channel formation in phospholipid bilayer by)

IT 5965-65-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction with benzyloxycarbonylethylenediamine

hydrochloride of)
IT 148526-31-2P 148526-32-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction with lactose derivs. of)
IT 3262-72-4
RL: RCT (Reactant)
(reaction of, with chloromethylanthracene and sodium hydride)
IT 18807-71-1, N-Benzyloxycarbonylethylenediamine hydrochloride
RL: RCT (Reactant)
(reaction of, with lactonolactone)
IT 7646-69-7, Sodium hydride
RL: RCT (Reactant)
(reaction of, with serine derivs. and chloromethylanthracene)
IT 24463-19-2, 9-Chloromethylanthracene
RL: RCT (Reactant)
(reaction of, with serine derivs. and sodium hydride)

L66 ANSWER 7 OF 10 HCAPLUS COPYRIGHT 2000 ACS
AN 1992:572078 HCAPLUS
DN 117:172078
TI Changes in conformation and antimicrobial properties caused by replacement of D-amino acids with .alpha.-aminoisobutyric acid in the gramicidin backbone: synthesis and circular dichroic studies
AU Jelokhani-Niaraki, Masood; Yoshioka, Katsumi; Takahashi, Hiroki; Kato, Fumio; Kondo, Michio
CS Fac. Sci. Eng., Saga Univ., Saga, 840, Japan
SO J. Chem. Soc., Perkin Trans. 2 (1992), (7), 1187-93
CODEN: JCPKBH; ISSN: 0300-9580
DT Journal
LA English
CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 10, 22
AB In an attempt to mimic the stable helical structures of proteins with possible pore-forming ability in membranes, the linear gramicidin backbone has been changed by inserting achiral .alpha.-aminoisobutyric acids (Aib) in place of all the alternatively sequenced D-amino acids. The conformation and biol. activity of the synthetic gramicidin A and B analogs have been studied. CD measurements have been used to det. the conformation in soln. The original conformation of gramicidin clearly changes and its antimicrobial activity is reduced in Aib analogs. Although .alpha.-helical motifs can be clearly distinguished in analogs, the CD spectra show inherent complexities. The possibility of superposition of different conformations is considered. The potential pore-forming ability of analogs is briefly discussed.
ST aminoisobutyric acid analog gramicidin conformation; structure activity bactericide gramicidin analog
IT Conformation and Conformers
(of .alpha.-aminoisobutyric acid-contg. gramicidin analogs)
IT Bactericides, Disinfectants, and Antiseptics
(.alpha.-aminoisobutyric acid-contg. gramicidin analogs)
IT Molecular structure-biological activity relationship
(bactericidal, of .alpha.-aminoisobutyric acid-contg. gramicidin analogs)
IT 1405-97-6P, Gramicidin
RL: SPN (Synthetic preparation); PREP (Preparation)
(aminoisobutyric acid-contg. analogs, prepn., conformation, and bactericidal activity of)
IT 1161-13-3, N-Benzyloxycarbonylphenylalanine 2002-24-6, 2-Aminoethanol hydrochloride 5680-79-5, Glycine methyl ester hydrochloride 7432-21-5 13734-41-3 15028-41-8, .alpha.-Aminoisobutyric acid methyl ester hydrochloride 15761-38-3, N-tert-Butoxycarbonylalanine
RL: RCT (Reactant)
(peptide coupling reactions of, in prepn. of gramicidin analogs)
IT 143868-49-9P 143868-66-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and catalytic hydrogenolysis)

IT 2637-44-7P 143868-54-6P 143868-61-5P 143868-68-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and catalytic hydrogenolysis of)
IT 66449-52-3P 143868-56-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and deblocking of, with hydrogen chloride)
IT 143868-62-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and deblocking of, with trifluoroacetic acid)
IT **143868-51-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and formylation of)
IT 143868-48-8P 143868-65-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and peptide coupling of, in prepn. of gramicidin analog)
IT 143868-47-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and peptide coupling of, in prepn. of gramicidin analogs)
IT 143868-53-5P 143868-67-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and peptide coupling of, with dipeptide deriv. in prepn. of gramicidin analog)
IT 1685-28-5P 85918-88-3P 89045-43-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and peptide coupling of, with dipeptide deriv. in prepn. of gramicidin analogs)
IT 143868-60-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and peptide coupling of, with dipeptide derivs. in prepn. of gramicidin analogs)
IT 45233-75-8P 72095-04-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and peptide coupling of, with dipeptide ester in prepn. of gramicidin analogs)
IT 143868-59-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and peptide coupling of, with tetrapeptide deriv. in prepn. of gramicidin analogs)
IT 143868-57-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and peptide coupling of, with tetrapeptide ester in prepn. of gramicidin analogs)
IT 109772-33-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and peptide coupling of, with tetrapeptide in prepn. of gramicidin analog)
IT 143868-52-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and peptide coupling reactions of, in prepn. of gramicidin analogs)
IT 51803-69-1P 98714-71-7P 143868-50-2P 143868-55-7P 143868-63-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and sapon. of)
IT 143868-46-6P 143868-64-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn., conformation, and bactericidal activity of)
IT 72086-77-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn., deblocking, or sapon. of)

L66 ANSWER 8 OF 10 HCAPLUS COPYRIGHT 2000 ACS
AN 1988:590816 HCAPLUS
DN 109:190816
TI Synthesis of linear undecapeptide precursors of cyclosporin analogs
AU Galpin, I. J.; Mohammed, A. K. A.; Patel, A.
CS Robert Robinson Lab., Univ. Liverpool, Liverpool, L69 3BX, UK

SO Tetrahedron (1988), 44(6), 1773-82
CODEN: TETRAB; ISSN: 0040-4020
DT Journal
LA English
CC 34-3 (Amino Acids, Peptides, and Proteins)
OS CASREACT 109:190816
AB Eleven protected undecapeptide precursors of cyclosporin analogs were prepd. by stepwise elongation of PhCH2O2C-(4-11)-OCMe3 using the diphenylphosphinic mixed anhydride method. Yields were in the 60-90% range and optically pure peptides were obtained. A no. of fragment condensations approaches were studied; the diphenylphosphinic anhydride fragment coupling gave only a 39% yield.
ST cyclosporin analog undecapeptide precursor
IT Peptides, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(undeca-, prepn. of, as precursors of cyclosporin analogs)
IT 28920-43-6
RL: RCT (Reactant)
(acylation by, of threonine deriv.)
IT 82911-69-1
RL: RCT (Reactant)
(fluorenylmethoxycarbonylation by, of diaminobutyric acid)
IT 1883-09-6 42417-72-1
RL: RCT (Reactant)
(fluorenylmethoxycarbonylation of)
IT 16966-09-9 42417-73-2 42918-86-5
RL: RCT (Reactant)
(peptide coupling of)
IT 39608-31-6
RL: RCT (Reactant)
(peptide coupling of with octapeptide deriv.)
IT 21691-44-1, N-Benzyloxycarbonyl-L-norvaline 39608-30-5, N-Benzyloxycarbonyl-L-norleucine
RL: RCT (Reactant)
(peptide coupling of, with nonapeptide deriv.)
IT 117106-30-6
RL: RCT (Reactant)
(peptide coupling of, with octapeptide deriv.)
IT **117106-24-8**
RL: RCT (Reactant)
(peptide coupling of, with sarcosine deriv.)
IT 117106-31-7
RL: RCT (Reactant)
(peptide coupling of, with tripeptide deriv.)
IT 116236-40-9P 116823-65-5P 117106-17-9P 117106-18-0P 117129-76-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and hydrogenolysis of)
IT 85201-91-8P 117106-19-1P 117106-20-4P 117106-21-5P 117106-25-9P 117106-26-0P 117106-27-1P 117106-28-2P 117106-29-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and peptide coupling of)
IT 117106-23-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and sapon. of)
IT 117106-22-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and tert-butoxycarbonylation of)
IT 116236-39-6P 116236-41-0P 116236-42-1P 116236-43-2P 116236-44-3P 116236-45-4P 116236-46-5P 116236-47-6P 116236-48-7P 116236-49-8P 116236-50-1P 116236-51-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
IT 79217-60-0DP, Cyclosporin, analogs
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of linear undecapeptide precursors of)
IT 1676-75-1

RL: RCT (Reactant)
(N-methylation of)
IT 115-11-7, Isobutylene, reactions
RL: RCT (Reactant)
(O-tert-butylation by, of hydroxyproline deriv.)
IT 112203-99-3
RL: RCT (Reactant)
(O-tert-butylation of, with isobutylene)

L66 ANSWER 9 OF 10 HCAPLUS COPYRIGHT 2000 ACS
AN 1986:104617 HCAPLUS
DN 104:104617
TI Vibrational circular dichroism of polypeptides, V. A study of 310-helical-octapeptides
AU Yasui, Sritana C.; Keiderling, Timothy A.; Bonora, Gian Maria; Toniolo, Claudio
CS Dep. Chem., Univ. Illinois, Chicago, IL, 60680, USA
SO Biopolymers (1986), 25(1), 79-89
CODEN: BIPMAA; ISSN: 0006-3525
DT Journal
LA English
CC 6-3 (General Biochemistry)
AB Vibrational CD spectra were measured in the 3600-1250 cm-1 region of 2 monodisperse, protected octapeptides which form right-handed 310-helixes in CDCl3 soln. The spectra are similar in sign pattern to those obtained for right-handed .alpha.-helixes in soln. but are smaller in magnitude and, addnl., provide evidence of some line-shape differences. The delineation of this type of ordered conformation was accomplished by means of 1H NMR. Such a soln. structure is consistent with the x-ray crystal structure of 1 of these mols.
ST vibrational CD peptide conformation; helix 3 10 protein vibrational CD
IT Peptides, properties
Proteins
RL: PRP (Properties)
(conformation of, 310-helical, vibrational CD in relation to)
IT Infrared spectra
Nuclear magnetic resonance
(of peptides, vibrational CD in relation to)
IT Conformation and Conformers
(310-helical, of proteins, vibrational CD in relation to)
IT Crystal structure-property relationship
(conformation, of peptides)
IT 72485-35-9
RL: RCT (Reactant)
(deprotection of)
IT 100817-47-8P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and vibrational CD spectra of, 310-helical conformation in relation to)
IT 90892-16-3
RL: RCT (Reactant)
(reaction of, with aminoisobutyrate polymer oxazolone)
IT 4512-43-0
RL: RCT (Reactant)
(reaction of, with leucylisobuteroaminoisobutyrate Me ester)
IT 95842-05-0 **100843-78-5**
RL: PRP (Properties)
(vibrational CD spectra of, 310-helical conformation in relation to)

L66 ANSWER 10 OF 10 HCAPLUS COPYRIGHT 2000 ACS
AN 1979:187312 HCAPLUS
DN 90:187312
TI Carbon-13 NMR spectroscopic studies on the conformation during stepwise synthesis of peptides bound to solubilizing polymer supports
AU Leibfritz, D.; Mayr, W.; Oekonomopulos, R.; Jung, G.
CS Inst. Org. Chem., Univ. Frankfurt, Frankfurt, Ger.

SO Tetrahedron (1978), 34(13), 2045-50
CODEN: TETRAB; ISSN: 0040-4020
DT Journal
LA English
CC 34-3 (Synthesis of Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 22, 35
AB The 13C (13C-1H) triple resonance technique was applied to constitutional and conformational studies of polypeptides bound to mono- and bifunctional solubilizing polyoxyethylene supports. High resoln. showed distinct differences between random coil and .alpha.-helical conformations. This method is valuable for the control of the growing peptide during stepwise synthesis on sol. polymeric supports. Examples of partial sequences of alamethicin and sequential analogs demonstrate the applicability to peptide polyoxyethylene esters with mean mol. wts. of 2000-10,000.
ST polyoxyethylene bound peptide conformation NMR; alamethicin conformation carbon NMR; Merrifield peptide prepn carbon NMR
IT Peptides, properties
RL: PRP (Properties)
(conformation of polymer-bound, carbon-13 NMR detn. of)
IT Merrifield synthesis
(of peptides, conformational control in, carbon-13 NMR in relation to)
IT Conformation and Conformers
(of polyoxyethylene-bound peptides, carbon-13 NMR detn. of)
IT Nuclear magnetic resonance
(carbon-13, in polyoxyethylene-bound peptides)
IT 13726-85-7D, polymer-bound 13734-41-3D, polymer-bound 32991-17-6D, polymer-bound 70134-38-2D, polymer-bound 70134-39-3D, polymer-bound 70134-40-6D, polymer-bound 70134-41-7D, polymer-bound 70134-42-8D, polymer-bound **70134-43-9D**, polymer-bound 70134-44-0D, polymer-bound
RL: PRP (Properties)
(conformation of, carbon-13 NMR detn. of)